10590399

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasxm1624

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS 1   Web Page for STN Seminar Schedule - N. America
 NEWS 2 JUN 06   EPFULL enhanced with 260,000 English abstracts
 NEWS 3 JUN 06   KOREAPAT updated with 41,000 documents
 NEWS 4 JUN 13   USPATFULL and USPAT2 updated with 11-character
                   patent numbers for U.S. applications
 NEWS 5 JUN 19   CAS REGISTRY includes selected substances from
                   web-based collections
 NEWS 6 JUN 25   CA/CAplus and USPAT databases updated with IPC
                   reclassification data
 NEWS 7 JUN 30   AEROSPACE enhanced with more than 1 million U.S.
                   patent records
 NEWS 8 JUN 30   EMBASE, EMBAL, and LEMBASE updated with additional
                   options to display authors and affiliated
                   organizations
 NEWS 9 JUN 30   STN on the Web enhanced with new STN AnaVist
                   Assistant and BLAST plug-in
 NEWS 10 JUN 30   STN AnaVist enhanced with database content from EPFULL
 NEWS 11 JUL 28   CA/CAplus patent coverage enhanced
 NEWS 12 JUL 28   EPFULL enhanced with additional legal status
                   information from the epoline Register
 NEWS 13 JUL 28   IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
 NEWS 14 JUL 28   STN Viewer performance improved
 NEWS 15 AUG 01   INPADOCDB and INPAFAMDB coverage enhanced
 NEWS 16 AUG 13   CA/CAplus enhanced with printed Chemical Abstracts
                   page images from 1967-1998
 NEWS 17 AUG 15   CAOLD to be discontinued on December 31, 2008
 NEWS 18 AUG 15   CAplus currency for Korean patents enhanced
 NEWS 19 AUG 27   CAS definition of basic patents expanded to ensure
                   comprehensive access to substance and sequence
                   information
 NEWS 20 SEP 18   Support for STN Express, Versions 6.01 and earlier,
                   to be discontinued
 NEWS 21 SEP 25   CA/CAplus current-awareness alert options enhanced
                   to accommodate supplemental CAS indexing of
                   exemplified prophetic substances
 NEWS 22 SEP 26   WPIDS, WPINDEX, and WPIX coverage of Chinese and
                   and Korean patents enhanced
 NEWS 23 SEP 29   IFICLS enhanced with new super search field
 NEWS 24 SEP 29   EMBASE and EMBAL enhanced with new search and
                   display fields
 NEWS 25 SEP 30   CAS patent coverage enhanced to include exemplified

                      prophetic substances identified in new Japanese-
                      language patents
NEWS 26 OCT 07 EPFULL enhanced with full implementation of EPC2000
NEWS 27 OCT 07 Multiple databases enhanced for more flexible patent
                      number searching
NEWS 28 OCT 22 Current-awareness alert (SDI) setup and editing
                      enhanced
NEWS 29 OCT 22 WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT
                      Applications

  NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
                  AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

  NEWS HOURS   STN Operating Hours Plus Help Desk Availability
  NEWS LOGIN   Welcome Banner and News Items
  NEWS IPC8   For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN Customer
  agreement. Please note that this agreement limits use to scientific
  research. Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:19:20 ON 23 OCT 2008

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                  ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'REGISTRY' ENTERED AT 12:19:41 ON 23 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 22 OCT 2008 HIGHEST RN 1064721-02-3
DICTIONARY FILE UPDATES: 22 OCT 2008 HIGHEST RN 1064721-02-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
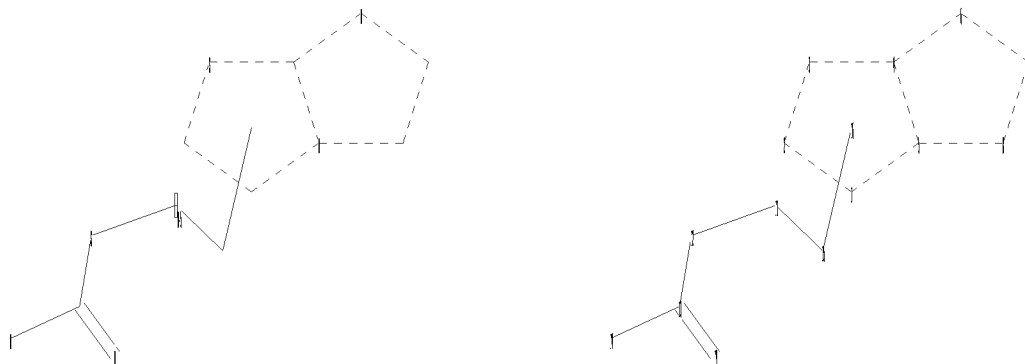 conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

10590399

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10590399.str

chain nodes :
11 12 13 14 15 19
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
11-12 11-15 12-13 13-14 13-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8 11-12 12-13 13-14 13-19
exact bonds :
11-15

G1:H,Cy,Ak

G2:H,X,Cy,Ak,CN,NO2,O,C

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:CLASS

L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR

10590399
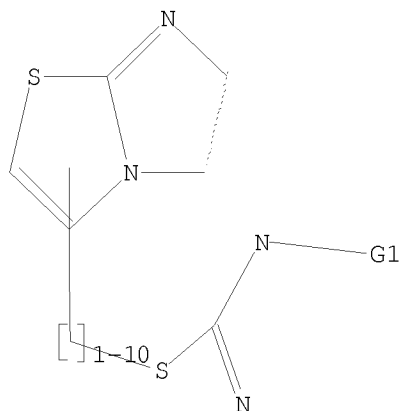
G1 H,Cy,Ak
G2 H,X,Cy,Ak,CN,NO2,O,C

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sam
SAMPLE SEARCH INITIATED 12:20:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   6 TO ITERATE

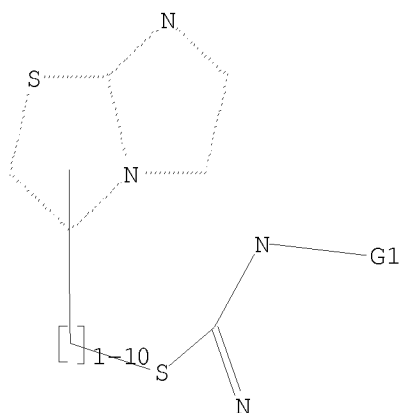100.0% PROCESSED   6 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 6 TO   266
PROJECTED ANSWERS: 0 TO   0

L2   0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 12:20:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   101 TO ITERATE

100.0% PROCESSED   101 ITERATIONS   0 ANSWERS
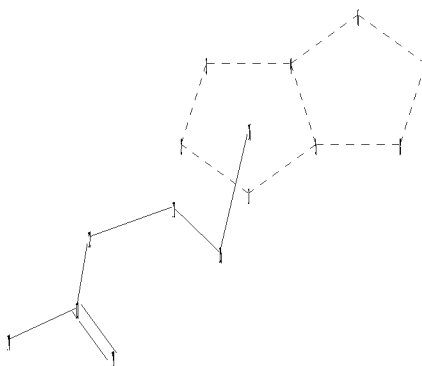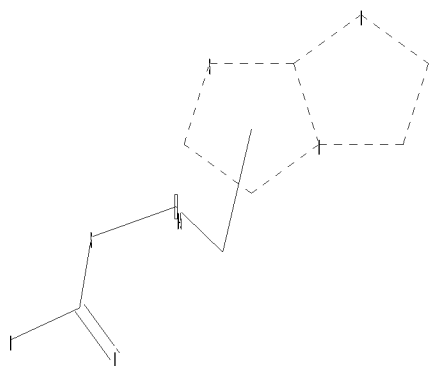SEARCH TIME: 00.00.01

L3   0 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10590399.str

10590399
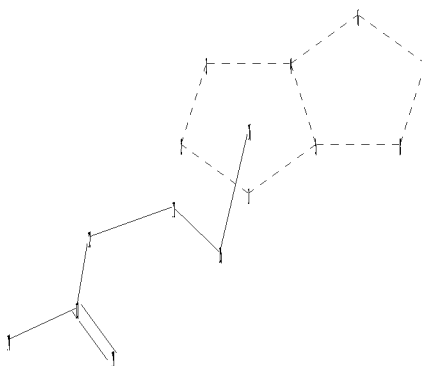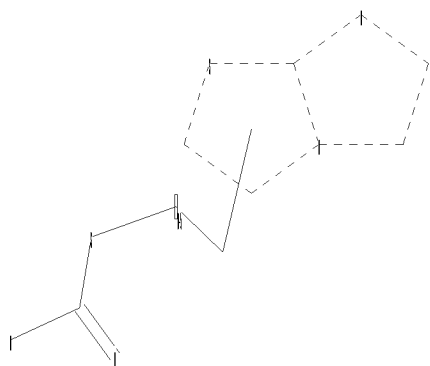

```
chain nodes :
11  12  13  14  15  19
ring nodes :
1  2  3  4  5  6  7  8
chain bonds :
11-12  11-15  12-13  13-14  13-19
ring bonds :
1-2  1-5  2-3  3-4  4-5  4-6  5-8  6-7  7-8
exact/norm bonds :
1-2  1-5  2-3  3-4  4-5  4-6  5-8  6-7  7-8  11-12  12-13  13-14  13-19
exact bonds :
11-15


G1:H,Cy,Ak

G2:H,X,Cy,Ak,CN,NO2,O,C

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  11:CLASS  12:CLASS
13:CLASS  14:CLASS  15:CLASS  16:CLASS  19:CLASS




L4        STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4                STR
```
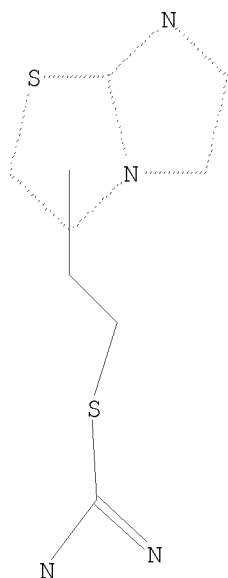
G1 H,Cy,Ak
G2 H,X,Cy,Ak,CN,NO2,O,C

Structure attributes must be viewed using STN Express query preparation.


```
=> s l4 sam
SAMPLE SEARCH INITIATED 12:21:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        6 TO ITERATE

100.0% PROCESSED        6 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          6 TO       266
PROJECTED ANSWERS:             0 TO         0

L5              0 SEA SSS SAM L4

=> s l4 ful
FULL SEARCH INITIATED 12:21:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      101 TO ITERATE

100.0% PROCESSED       101 ITERATIONS                            0 ANSWERS
SEARCH TIME: 00.00.01

L6              0 SEA SSS FUL L4

=>
Uploading C:\Program Files\Stnexp\Queries\10590399.str
```
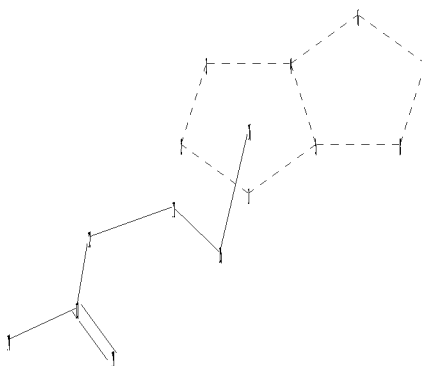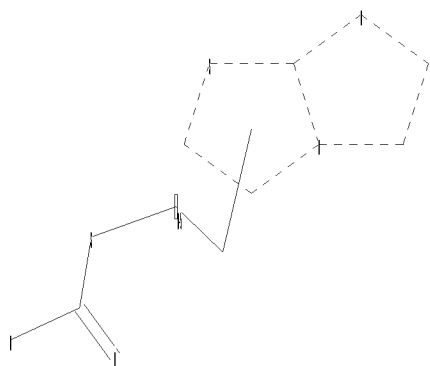
chain nodes :
11 12 13 14 15 19
ring nodes :
1   2   3   4   5   6   7   8
chain bonds :
11-12 11-15 12-13 13-14 13-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8 11-12 12-13 13-14 13-19
exact bonds :
11-15

G1:H,Cy,Ak

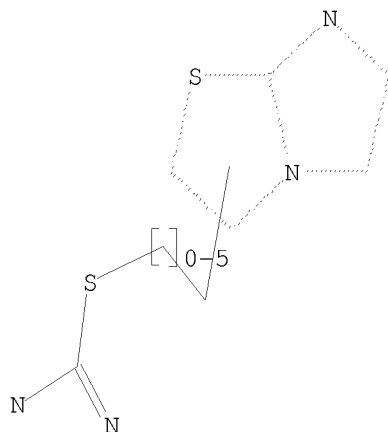G2:H,X,Cy,Ak,CN,NO2,O,C

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:CLASS

L7   STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7   STR

G1 H,Cy,Ak
G2 H,X,Cy,Ak,CN,NO2,O,C

Structure attributes must be viewed using STN Express query preparation.

=> s l7 sam
SAMPLE SEARCH INITIATED 12:23:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   6 TO ITERATE

100.0% PROCESSED   6 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 6 TO   266
PROJECTED ANSWERS: 0 TO   0

L8   0 SEA SSS SAM L7

=> s l7 ful
FULL SEARCH INITIATED 12:23:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   101 TO ITERATE

100.0% PROCESSED   101 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

L9   0 SEA SSS FUL L7

=>
Uploading C:\Program Files\Stnexp\Queries\10590399.str

chain nodes :
11 12 13 14 15 19
ring nodes :
1 2 3 4 5 6 7 8
chain bonds :
11-12 11-15 12-13 13-14 13-19
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-8 6-7 7-8 11-12 12-13 13-14 13-19
exact bonds :
11-15

G1:H,Cy,Ak

G2:H,X,Cy,Ak,CN,NO2,O,C

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:CLASS 19:CLASS

L10   STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10   STR

G1 H,Cy,Ak
G2 H,X,Cy,Ak,CN,NO2,O,C

Structure attributes must be viewed using STN Express query preparation.


```
=> s l10
SAMPLE SEARCH INITIATED 12:25:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        6 TO ITERATE

100.0% PROCESSED        6 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          6 TO       266
PROJECTED ANSWERS:             1 TO        80

L11            1 SEA SSS SAM L10

=> s l10 ful
FULL SEARCH INITIATED 12:25:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      101 TO ITERATE

100.0% PROCESSED       101 ITERATIONS                            25 ANSWERS
SEARCH TIME: 00.00.01

L12           25 SEA SSS FUL L10

=> fil capl
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY      SESSION
FULL ESTIMATED COST                                 716.20       716.41

FILE 'CAPLUS' ENTERED AT 12:25:42 ON 23 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
```

10590399

FILE COVERS 1907 - 23 Oct 2008 VOL 149 ISS 17
FILE LAST UPDATED: 22 Oct 2008 (20081022/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

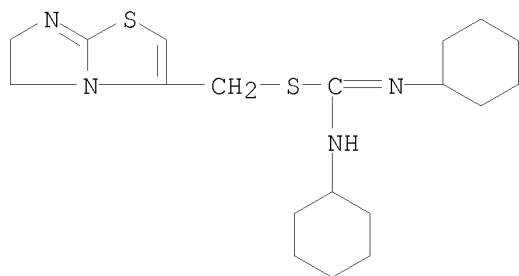http://www.cas.org/legal/infopolicy.html

=> s l12
L13   2 L12

=> d l13 ibib hitstr abs 1-2

L13   ANSWER 1 OF 2   CAPLUS   COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:201770 CAPLUS
DOCUMENT NUMBER: 146:244313
TITLE: CXCR4 binding molecules in treatment of WHIM syndrome
INVENTOR(S):   Kovarik, Jiri; Thoma, Gebhard; Weidmann, Beat; Wright,
                           Timothy; Zerwes, Hans-Guenter
PATENT ASSIGNEE(S):   Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE: PCT Int. Appl., 22pp.
                           CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
        ---------------   ----   -------- --------------------   --------
        WO 2007022385   A2   20070222 WO 2006-US32192   20060817
        WO 2007022385   A3   20071101
            W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
                 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
                 GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP,
                 KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN,
                 MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
                 RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
                 UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
            RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
                 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
                 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
                 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
                 KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
        EP 1924260   A2   20080528 EP 2006-801766   20060817
            R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
                 IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,
                 BA, HR, MK, RS
        US 20080234294   A1   20080925 US 2008-64068   20080218
PRIORITY APPLN. INFO.:   US 2005-709399P   P   20050818
                                               WO 2006-US32192   W   20060817
OTHER SOURCE(S):   MARPAT 146:244313
IT   864677-52-1 864677-55-4 864677-62-3
     864677-63-4 864677-67-8 864677-68-9
     864677-69-0 864677-76-9
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (CXCR4 binding mols. in treatment of WHIM syndrome)
RN   864677-52-1 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclohexyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)
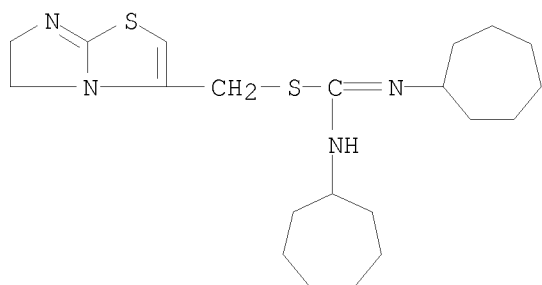
RN   864677-55-4 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclohexyl-,
      (5,6-dihydro-6,6-dimethylimidazo[2,1-b]thiazol-3-yl)methyl ester (CA
      INDEX NAME)
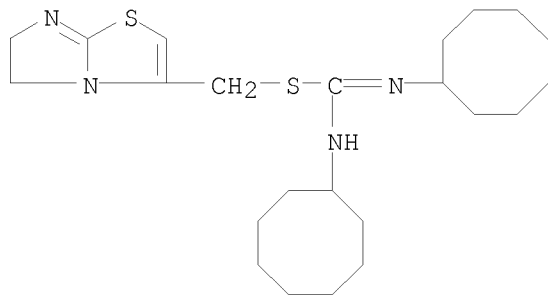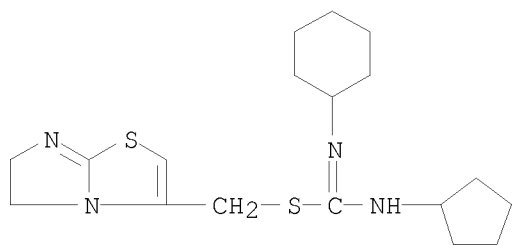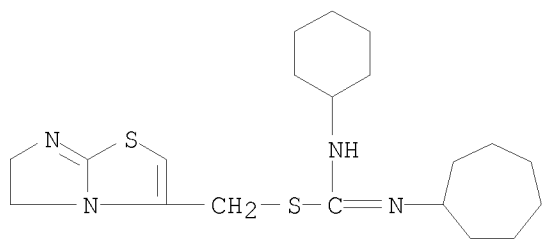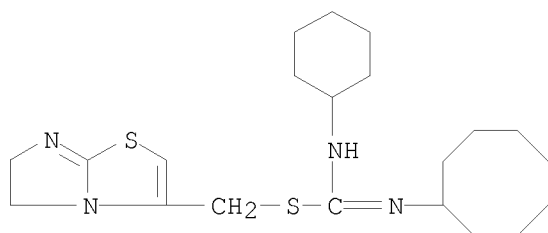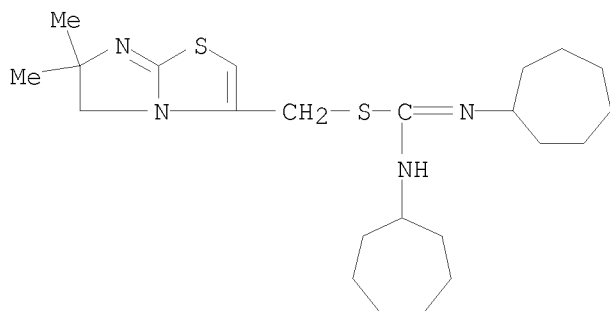

RN   864677-62-3 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicycloheptyl-,
      (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester (CA INDEX NAME)

RN   864677-63-4 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclooctyl-,
      (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester (CA INDEX NAME)

RN   864677-67-8   CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-cyclopentyl-,
      (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-68-9   CAPLUS
CN   Carbamimidothioic acid, N-cycloheptyl-N'-cyclohexyl-,
      (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-69-0   CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-cyclooctyl-,
      (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-76-9   CAPLUS
CN   Carbamimidothioic acid, N,N'-dicycloheptyl-,
     (5,6-dihydro-6,6-dimethylimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA
     INDEX NAME)

AB   This invention relates to the use of a CXCR-binding mols. as described in
     the specification, in Warts-Hypogammaglobulinemia-Immunodeficiency-
     Myelokathexis (WHIM) syndrome.

```
L13  ANSWER 2 OF 2  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:          2005:1004725  CAPLUS
DOCUMENT NUMBER:           143:306301
TITLE:                     Preparation of thiazolyl isothiourea derivatives as
                           CXCR4 antagonists
INVENTOR(S):               Glickman, Fraser; Streiff, Markus; Thoma, Gebhard;
                           Zerwes, Hans-Guenter
PATENT ASSIGNEE(S):        Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE:                    PCT Int. Appl., 34 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE:             Patent
LANGUAGE:                  English
FAMILY ACC. NUM. COUNT:    1
PATENT INFORMATION:

        PATENT NO.           KIND   DATE       APPLICATION NO.        DATE
        ---------------      ----   --------   --------------------   --------
        WO 2005085219        A1     20050915   WO 2005-EP2014         20050225
            W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
                CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
                GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
                LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
                NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
                SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
            RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
                AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
                EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
                RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
                MR, NE, SN, TD, TG
        AU 2005219531        A1     20050915   AU 2005-219531         20050225
        CA 2556386           A1     20050915   CA 2005-2556386        20050225
        EP 1720845           A1     20061115   EP 2005-715554         20050225
            R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
                IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR
        CN 1922158           A      20070228   CN 2005-80006094       20050225
        JP 2007523941        T      20070823   JP 2007-500168         20050225
        MX 2006PA09696       A      20061120   MX 2006-PA9696         20060825
        IN 2006CN03099       A      20070608   IN 2006-CN3099         20060825
        US 20070161618       A1     20070712   US 2006-590399         20060926
PRIORITY APPLN. INFO.:                         GB 2004-4434      A    20040227
                                               WO 2005-EP2014    W    20050225
OTHER SOURCE(S):           CASREACT 143:306301; MARPAT 143:306301
IT   864677-52-1P 864677-55-4P 864677-56-5P
     864677-58-7P 864677-59-8P 864677-60-1P
     864677-61-2P 864677-62-3P 864677-63-4P
     864677-64-5P 864677-65-6P 864677-66-7P
     864677-67-8P 864677-68-9P 864677-69-0P
     864677-70-3P 864677-71-4P 864677-72-5P
     864677-73-6P 864677-74-7P 864677-75-8P
     864677-76-9P 864677-79-2P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of thiazolyl isothiourea derivs. as CXCR4 antagonists)
RN   864677-52-1  CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclohexyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester  (CA INDEX NAME)
```
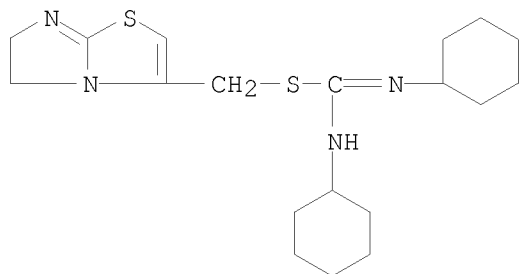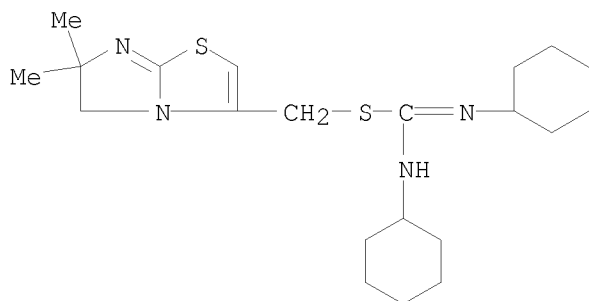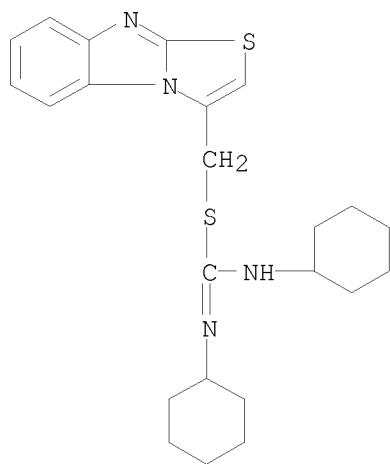
10590399

RN   864677-55-4 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclohexyl-,
      (5,6-dihydro-6,6-dimethylimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA
      INDEX NAME)

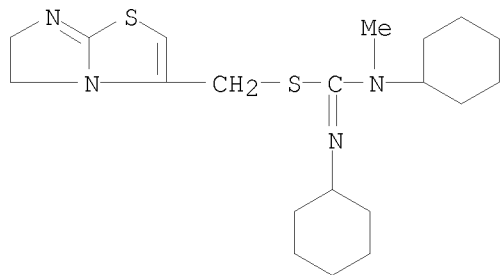RN   864677-56-5 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclohexyl-,
      thiazolo[3,2-a]benzimidazol-3-ylmethyl ester   (CA INDEX NAME)
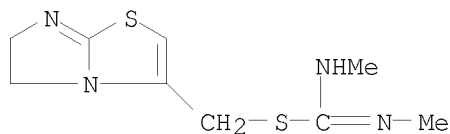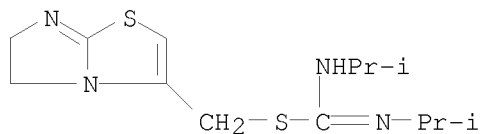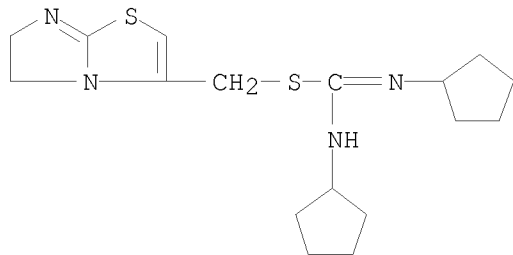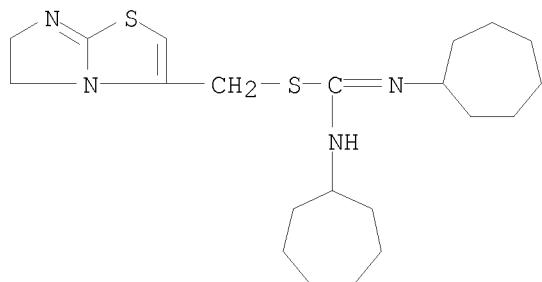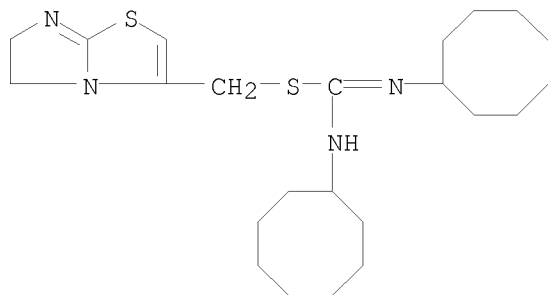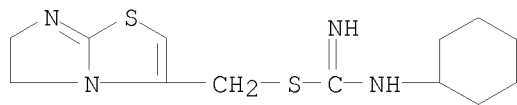

RN   864677-58-7 CAPLUS

10590399

CN   Carbamimidothioic acid, N,N'-dicyclohexyl-N-methyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

CH2—S—C—N—Cyclohexyl structure with Me and N-cyclohexyl

RN   864677-59-8   CAPLUS
CN   Carbamimidothioic acid, N,N'-dimethyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)
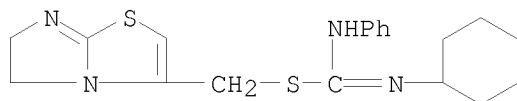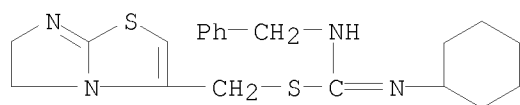
CH2—S—C(NHMe)=N—Me structure

RN   864677-60-1   CAPLUS
CN   Carbamimidothioic acid, N,N'-bis(1-methylethyl)-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

CH2—S—C(NHPr-i)=N—Pr-i structure

RN   864677-61-2   CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclopentyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

CH2—S—C(=N—cyclopentyl)(NH—cyclopentyl) structure

RN   864677-62-3   CAPLUS

10590399

CN   Carbamimidothioic acid, N,N'-dicycloheptyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-63-4 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclooctyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

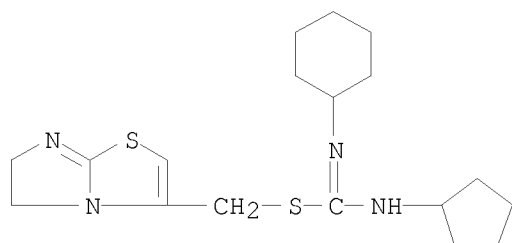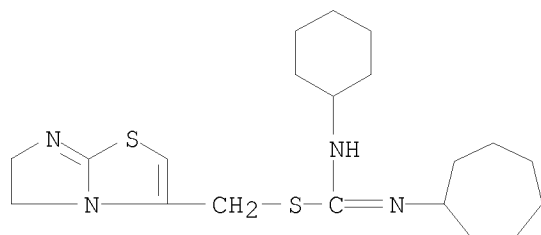RN   864677-64-5 CAPLUS
CN   Carbamimidothioic acid, cyclohexyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester (9CI)   (CA INDEX NAME)

RN   864677-65-6 CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-phenyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-66-7 CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-(phenylmethyl)-,

(5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-67-8   CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-cyclopentyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)
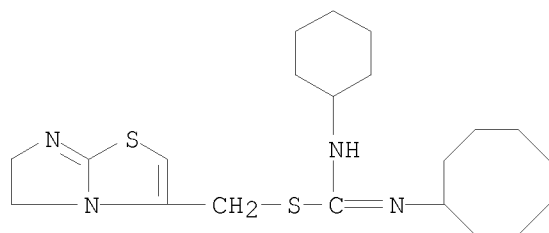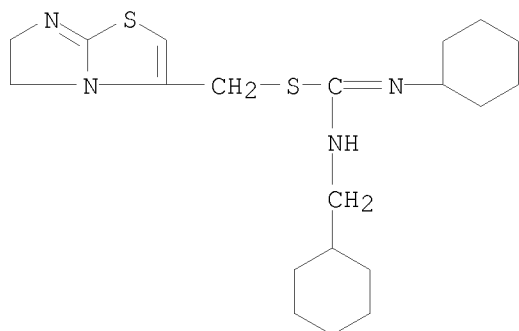

RN   864677-68-9   CAPLUS
CN   Carbamimidothioic acid, N-cycloheptyl-N'-cyclohexyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-69-0   CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-cyclooctyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-70-3   CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-(cyclohexylmethyl)-,
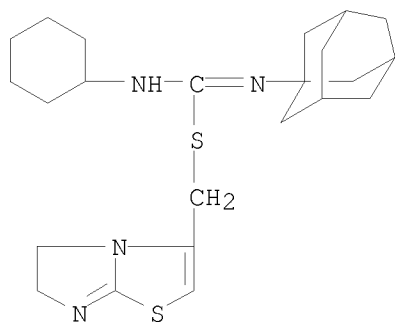
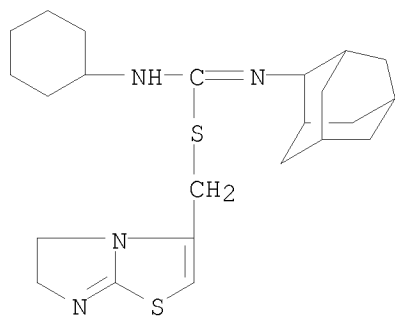(5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-71-4 CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-tricyclo[3.3.1.13,7]dec-1-yl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)
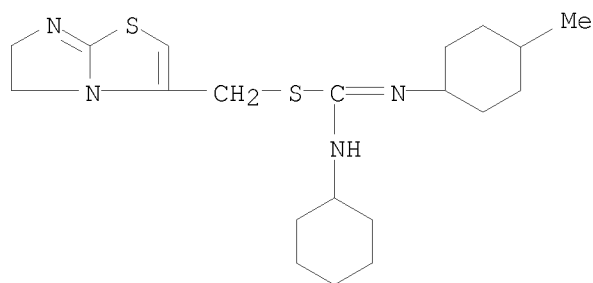

RN   864677-72-5 CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-tricyclo[3.3.1.13,7]dec-2-yl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)
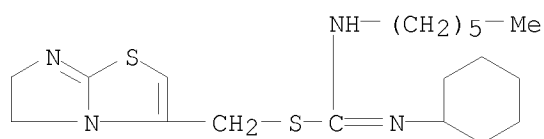

RN   864677-73-6 CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-(4-methylcyclohexyl)-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)
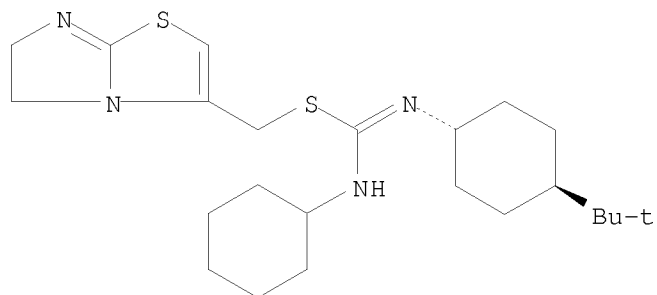
RN   864677-74-7 CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-hexyl-,
     (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA INDEX NAME)

RN   864677-75-8 CAPLUS
CN   Carbamimidothioic acid, N-cyclohexyl-N'-[trans-4-(1,1-
     dimethylethyl)cyclohexyl]-, (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl
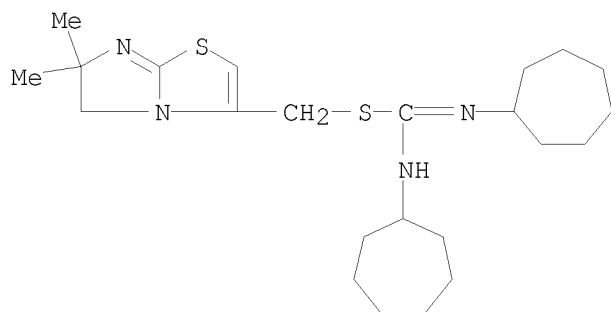   ester   (CA INDEX NAME)

Relative stereochemistry.

RN   864677-76-9 CAPLUS
CN   Carbamimidothioic acid, N,N'-dicycloheptyl-,
     (5,6-dihydro-6,6-dimethylimidazo[2,1-b]thiazol-3-yl)methyl ester   (CA
     INDEX NAME)

Me
Me

N   S

N   CH₂—S—C=N—(cycloheptyl)

NH

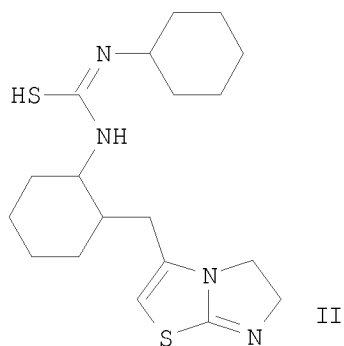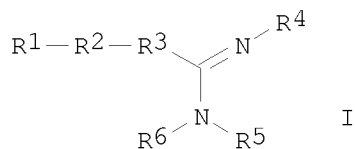(cycloheptyl)

RN   864677-79-2   CAPLUS
CN   Carbamimidothioic acid, N,N'-dicyclohexyl-,
      (5,6-dihydroimidazo[2,1-b]thiazol-3-yl)methyl ester, dihydrochloride (9CI)
        (CA INDEX NAME)

N   S

N   CH₂—S—C=N—(cyclohexyl)

NH

(cyclohexyl)

●2 HCl

GI

I
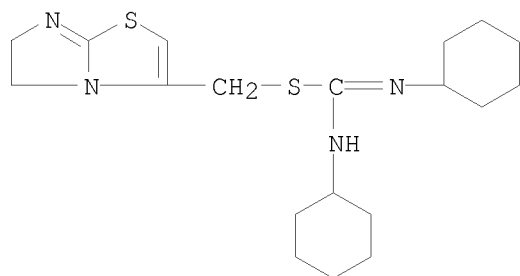
II

AB   Title compds. I [R1 = (un)substituted pyrrolidine or pyrimidinyl
      pyrrolidine; R2 = CO or (CR7R8)1-3; R3 = S, O or NR9; R4 and R5
      independently = (un)substituted cycloalkyl, alkyl, aryl, etc.; R6 = H,
      alkyl, cycloalkyl, etc.; R7 and R8 independently = H, F, Cl, etc.; R9 = H,
      alkoxyalkyl, haloalkyl, etc.] and their pharmaceutically acceptable salts,
      are prepared and disclosed as antagonists of CXCR4. Thus, e.g., II was
      prepared by coupling of N,N'-dicyclohexyl thiourea with
      3-chloromethyl-5,6-dihydroimidazo[2,1-b]thiazole. The activity of I was
      evaluated in a CXCR4 membrane binding assay and it was revealed that
      compds. of the invention displayed an IC50 value of <50 μM. I as
      antagonist of CXCR4 should prove useful in the treatment of transplant
      rejection, inflammatory diseases and infectious diseases, in particular
      progression of AIDS. Pharmaceutical compns. comprising I are disclosed.
REFERENCE COUNT: 15   THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10590399

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.38	727.79

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.60	-1.60

STN INTERNATIONAL LOGOFF AT 12:26:26 ON 23 OCT 2008